(FILE 'HOME' ENTERED AT 16:25:57 ON 10 NOV 2004)

FILE 'CAPLUS' ENTERED AT 16:31:09 ON 10 NOV 2004
L1 0 S (PROTEIN AND (FORCEFIELD OR (FORCEFIELD)) AND CALCULATION#)/T
L2 8 S (PROTEIN AND (FORCEFIELD OR (FORCE FIELD)) AND CALCULATION#)/

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L2 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:224327 CAPLUS
TI **Protein force field** parameterization by free energy **calculations**
AU Guvench, Olgun; Brooks, Charles L.
CS Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), COMP-178 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69FGKM
DT Conference; Meeting Abstract
LA English
AB Mol. dynamics simulations of proteins which include explicit representation of water mols. continue to be very time consuming despite advances in computer hardware. In an effort to reach longer timescales, we have developed a simple energy function for protein modeling which includes only bonded, volume exclusion, length scale dependent hydrophobicity, and hydrogen bonding terms. To parameterize the model we employ methods of statistical mechanics to calculate free energies for hydrophobic chain collapse and protein folding. The resulting parameters combined with the energy function yield a force field which favors near-native structures for small all-alpha, all-beta, and mixed alpha/beta proteins and which is more than two orders of magnitude faster than explicit water simulations.

L2 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:888339 CAPLUS
DN 140:107714
TI A point-charge **force field** for molecular mechanics simulations of **proteins** based on condensed-phase quantum mechanical **calculations**
AU Duan, Yong; Wu, Chun; Chowdhury, Shibasish; Lee, Mathew C.; Xiong, Guoming; Zhang, Wei; Yang, Rong; Cieplak, Piotr; Luo, Ray; Lee, Taisung; Caldwell, James; Wang, Junmei; Kollman, Peter
CS Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716, USA
SO Journal of Computational Chemistry (2003), 24(16), 1999-2012
CODEN: JCCHDD; ISSN: 0192-8651
PB John Wiley & Sons, Inc.
DT Journal
LA English
AB Mol. mechanics models have been applied extensively to study the dynamics of proteins and nucleic acids. Here we report the development of a third-generation point-charge all-atom force field for proteins. Following the earlier approach of Cornell et al., the charge set was obtained by fitting to the electrostatic potentials of dipeptides calculated using B3LYP/cc-pVTZ/HF/6-31G** quantum mech. methods. The main-chain torsion parameters were obtained by fitting to the energy profiles of Ace-Ala-Nme and Ace-Gly-Nme di-peptides calculated using MP2/cc-pVTZ//HF/6-31G** quantum mech. methods. All other parameters were taken from the existing AMBER data base. The major departure from previous force fields is that all quantum mech. calcns. were done in the condensed phase with continuum solvent models and an effective dielec. constant of $\varepsilon = 4$. We anticipate that this force field parameter set will address certain

critical short comings of previous force fields in condensed-phase simulations of proteins. Initial tests on peptides demonstrated a high-degree of similarity between the calculated and the statistically measured Ramanchandran maps for both Ace-Gly-Nme and Ace-Ala-Nme di-peptides. Some highlights of our results include (1) well-preserved balance between the extended and helical region distributions, and (2) favorable type-II poly-proline helical region in agreement with recent expts. Backward compatibility between the new and Cornell et al. charge sets, as judged by overall agreement between dipole moments, allows a smooth transition to the new force field in the area of ligand-binding calcns. Test simulations on a large set of proteins are also discussed.
RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:689434 CAPLUS
DN 139:304087
TI Extremely precise free energy **calculations** of amino acid side chain analogs: Comparison of common molecular mechanics **force fields** for **proteins**
AU Shirts, Michael R.; Pitera, Jed W.; Swope, William C.; Pande, Vijay S.
CS Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA
SO Journal of Chemical Physics (2003), 119(11), 5740-5761
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
AB Quant. free energy computation involves both using a model that is sufficiently faithful to the exptl. system under study (accuracy) and establishing statistically meaningful measures of the uncertainties resulting from finite sampling (precision). We use large-scale distributed computing to access sufficient computational resources to extensively sample mol. systems and thus reduce statistical uncertainty of measured free energies. In order to examine the accuracy of a range of common models used for protein simulation, we calculate the free energy of hydration of 15 amino acid side chain analogs derived from recent versions of the OPLS-AA, CHARMM, and AMBER parameter sets in TIP3P water using thermodn. integration. We achieve a high degree of statistical precision in our simulations, obtaining uncertainties for the free energy of hydration of 0.02-0.05 kcal/mol, which are in general an order of magnitude smaller than those found in other studies. Notably, this level of precision is comparable to that obtained in exptl. hydration free energy measurements of the same mols. Root mean square differences from experiment over the set of mols. examined using AMBER-, CHARMM-, and OPLS-AA-derived parameters were 1.35 kcal/mol, 1.31 kcal/mol, and 0.85 kcal/mol, resp. Under the simulation conditions used, these force fields tend to uniformly underestimate solubility of all the side chain analogs. The relative free energies of hydration between amino acid side chain analogs were closer to experiment but still exhibited significant deviations. Although extensive computational resources may be needed for large nos. of mols., sufficient computational resources to calculate precise free energy calcns. for small mols. are accessible to most researchers.
RE.CNT 100 THERE ARE 100 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:181834 CAPLUS
TI A point-charge **force field** for molecular mechanics simulations of **proteins** based on condensed-phase quantum mechanical **calculations**
AU Duan, Yong; Chowdhury, Shibasish; Wu, Chun; Xiong, Guoming; Zhang, Wei; Yang, Rong; Lee, Matthew; Cieplak, Piotr; Luo, Ray; Lee, Taisung; Caldwell, James; Wang, Junmei; Kollman, Peter A.

CS Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716, USA
SO Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), COMP-147 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69DSA4
DT Conference; Meeting Abstract
LA English
AB The development of a point-charge all-atom force field parameter set is reported. A hallmark of this force field is that all quantum mech. calcns. were done in the condensed phase with continuum solvent models. Initial tests on peptides that can form well-defined secondary structures are presented. The successes on both alpha-helixes and beta-sheets strongly suggest that the force field has achieved a good balance between these two important conformations.

L2 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:276227 CAPLUS
DN 135:42446
TI Evaluation and Reparametrization of the OPLS-AA **Force Field** for **Proteins** via Comparison with Accurate Quantum Chemical **Calculations** on Peptides
AU Kaminski, George A.; Friesner, Richard A.; Tirado-Rives, Julian; Jorgensen, William L.
CS Department of Chemistry and Center for Biomolecular Simulation, Columbia University, New York, NY, 10027, USA
SO Journal of Physical Chemistry B (2001), 105(28), 6474-6487
CODEN: JPCBFK; ISSN: 1089-5647
PB American Chemical Society
DT Journal
LA English
AB We present results of improving the OPLS-AA force field for peptides by means of refitting the key Fourier torsional coeffs. The fitting technique combines using accurate ab initio data as the target, choosing an efficient fitting subspace of the whole potential-energy surface, and determining wts. for each of the fitting points based on magnitudes of the potential-energy gradient. The average energy RMS deviation from the LMP2/cc-pVTZ(-f)//HF/6-31G** data is reduced by .apprx.40% from 0.81 to 0.47 kcal/mol as a result of the fitting for the electrostatically uncharged dipeptides. Transferability of the parameters is demonstrated by using the same alanine dipeptide-fitted backbone torsional parameters for all of the other dipeptides (with the appropriate side-chain refitting) and the alanine tetrapeptide. Parameters of nonbonded interactions have also been refitted for the sulfur-containing dipeptides (cysteine and methionine), and the validity of the new Coulombic charges and the van der Waals σ's and ε's is proved through reproducing gas-phase energies of complex formation heats of vaporization and densities of pure model liqs. Moreover, a novel approach to fitting torsional parameters for electrostatically charged mol. systems has been presented and successfully tested on five dipeptides with charged side chains.
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:55332 CAPLUS
DN 126:191384
TI **Calculation** of **protein**-polymer **force fields** using molecular dynamics
AU Pitt, William G.; Weaver, Daniel R.
CS Chemical Engineering Dep., Brigham Young Univ., Provo, UT, 84602, USA
SO Journal of Colloid and Interface Science (1997), 185(1), 258-264
CODEN: JCISA5; ISSN: 0021-9797
PB Academic

DT Journal
LA English
AB Mol. dynamics simulations were performed to determine the force field of attraction between Leu-enkephalin and a model polyethylene surface. Four sep. rotational orientations of the polypeptide were simulated. During the simulations the surface atoms were held static, but the H2O atoms were dynamic. Some simulations were studied using restricted dynamics of the polypeptide in which only the 5 backbone α-carbon atoms held immobile. For an orientation with O atoms toward the PE surface, the force between the enkephalin and the surface was repulsive and was approaching zero as the separation reached 8 Å. The maximum repulsive force reached 8 kcal mol-1 Å-1 at 2.7 Å separation For an orientation with hydrophobic groups toward the PE, the force was attractive with a min. in the force field of 4 kcal mol-1 Å-1 at 2.3 Å. Two other orientations were also studied. The results of the MD simulations indicate that the force between enkephalin and PE in the region $0 < z < 9.5$ Å mostly is a function of the separation distance and the orientation angle of enkephalin with respect to the surface.
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:436678 CAPLUS
DN 125:108215
TI Position-dependent **protein** mutant profile based on mean **force field calculation**
AU Wang, Yanli; Lai, Luhua; Li, Shuwei; Han, Yuzhaen; Tang, Youqi
CS Inst. Phys. Chem., Peking Univ., Beijing, 100871, Peop. Rep. China
SO Protein Engineering (1996), 9(6), 479-484
CODEN: PRENE9; ISSN: 0269-2139
PB Oxford University Press
DT Journal
LA English
AB The application of the mean force field in protein mutant stability prediction is explored. Based on protein main chain characteristics, including polar fraction, accessibility and dihedral angles, the mean force field was constructed to evaluate the compatibility between an amino acid residue and its environment, from which a position-dependent protein mutant profile was constructed. At each position along a protein sequence, the native residue was replaced by the other 19 types of amino acid residues. The matches were evaluated by energies from mean force field calcn., from which a mutant profile along the protein sequence was derived. General characteristics of such a profile were analyzed. Mutant stabilities for two sets of mutants in two proteins were found to be reasonable compared with exptl. data, which indicates that the present method can act as a guide in protein engineering and as an effective scoring matrix in protein sequence-structure alignment studies.

L2 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:67206 CAPLUS
DN 118:67206
TI MM **calculations** of the metal-**protein** model complexes. I. Molecular **force field** for cobalt complexes
AU Cao, Wei Liang; Guo, Hong You; Xue, Shi Lei; Ren, Xin Gang; Wang, Zuo Xing
CS Beijing Inst. Chem. Technol., Beijing, 100029, Peop. Rep. China
SO Chinese Chemical Letters (1992), 3(5), 393-6
CODEN: CCLEE7; ISSN: 1001-8417
DT Journal
LA English
AB The structure of the model mol., Co(H2O)3SO4(phen) was studied by mol. mechanics. Mol. force field (MM2) parameters were developed for the particular class of the complexes.